Role of semi core levels in determining the band-gaps of semiconductors : First-principles calculations with model Hamiltonians

Roby Cherian[1], Priya Mahadevan[1] and Clas Persson[2]

[1] *S.N. Bose National Centre for Basic Sciences,*

JD-Block, Sector III,

Salt Lake, Kolkata-700098, India

[2] *Department of Materials Science and Engineering,*

Royal Institute of Technology,

SE-10044, Stockholm, Sweden

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Abstract

First principle calculations based on LDA/GGA approximation for the exchange functional underestimate the position of the semi core $3d$ levels in GaX (X=N, P and As) semiconductors. A self-interaction correction scheme within the LDA+U/GGA+U approximation is found to be sufficient to correct this discrepancy. A consequence of this correction is that the bandgap (E_g) of the semiconductors also improves. The belief has been that the bandgap correction comes from modified semi core-valence interaction. We examine this often used approximation in great detail and find that although bandgap changes as large as 0.63 eV for GaAs, 0.42 eV for GaP and 0.46 eV for GaN are obtained within this approach for U= 20 eV on the Ga d states, only 0.1 eV, 0.1 eV and 0.15 eV for GaAs, GaP and GaN arise from semi core-valence interaction. As U is increased, the bandgap keeps improving. We trace this effect primarily to the interaction of the Ga $4d$ states in the conduction band with the anion p states.

PACS numbers:

I. Introduction

Enormous progress has been made over the years in the development of realistic theories of materials starting from a first-principles approach [1]. A popular method in this direction is the Kohn-Sham formalism of density functional theory. The Hohenberg-Kohn theorem states [2] that the ground state energy can be written as an exact functional of the density. Unfortunately, the exact form of the functional is not known and approximations such as the local density approximation (LDA) [3, 4] as well as the generalised gradient approximation (GGA) [5, 6] have been used quite successfully in describing the ground state properties of a wide variety of systems. There are however limitations of this method when one attempts to calculate the excited state properties such as the bandgap. The Kohn-Sham band-gaps of semiconductors are smaller than the experimental values. Even if one ignores the fact that the Hohenberg-Kohn theorem is a theory of the ground state, there are limitations coming from the form of the exchange correlation functional. The Kohn-Sham (KS) band-gap E_g^{KS} is related to the fundamental band-gap of the solid E_g by the relation $E_g = E_g^{KS} + \Delta_{xc} + \Delta_U$ where Δ_{xc} is the discontinuity in the exchange correlation functional [7] when an electron is added to the system. and Δ_U has the corrections due to correlation effects. This discontinuity is lacking in the local density approximation resulting in the equality of the Kohn-Sham and the fundamental bandgap. The second, separate issue is the effect of the approximation of the exchange functional which arises from a spurious self-interaction error [4]. In addition electron correlation effects are underestimated in density functional theory which leads to the incorrect placement of the levels. For a more detailed discussion of the pros and cons of density functional theory see Ref [8].

For $s-p$ bonded semiconductors, the GW approximation [9] has been enormously successful in improving the calculated bandgap. In this method, a partially or fully self-consistent solution of the Dyson equation is used to determine the self-energy which provides a correction to the KS-LDA bandgap. Another contributory factor to the gap error is the cation d position in $s-p$ semiconductors [10], especially when these levels are relatively shallow. The d levels are not deep enough to be chemically inert and so they interact with the valence band states leading to a reduction of the bandgap. A cheap and rather inexpensive method that has been used in the literature [11, 12] for correcting for the bandgap has been the LDA+U/GGA+U method [13, 14]. Within this scheme a potential is introduced on the valence / semi core states which is dependent on the atom and angular momentum pro-

jected density operator. This pushes the semi core /valence states to deeper energies and therefore modifies the valence band maximum (VBM) position as a result of the modified semi core-valence / valence interaction.

In this work we have performed a detailed analysis of the GGA+U approach for correcting the bandgap of semiconductors in which a U is applied to the cation d states. We also studied the changes in the band structure and bandgap as a function of U. Aligning all the states with respect to the anion $1s$ level for that U value, we find that at Γ point, apart from movement of the Ga $3d$ states, the changes are primarily at the valence band maximum. All other states largely remain unshifted. As the semi core states are pushed to deeper energies, there would be a corresponding reduction in the coupling between the semi core and valence states. Hence for largish values of the U, the VBM should stop moving. This however does not happen. We examined if this was a consequence of the fact that the potential is angular momentum dependent, but does not distinguish between the 'principal quantum number' of the state involved. Invoking a description of the eigenfunctions in terms of an atomic description, for GaAs, the potential applied on the Ga d states does not distinguish between Ga $3d$ and Ga $4d$ states. There is a small admixture of the unoccupied Ga $4d$ states in the ground state charge density. The applied potential which depends on the Ga d density for a given value of U, pulls the Ga $4d$ states to lower energies where they interact more strongly with the As p states, therefore increasing the gap. This effect can be controlled by varying the muffin tin radius (RMT) of the sphere about Ga in which the potential is applied. A decreased muffin tin radius would have a reduced Ga $4d$ component and therefore modifies the potential. *However even after reducing the Ga 4d component*, the gap keeps increasing although the changes are small. These changes we speculate could arise from modified screening of the p states as the d states are moved deeper in energy or other modifications in the electronic structure arising from charge reorganization within the Ga states. For the first time we clarify how the bandgap is modified by a U on the semi core d states. We also provide the band offsets between the U=0 and finite U results for the GaX. These show that the self-interaction error due to the incorrect placement of the Ga d states changes both the valence band offset as well as the conduction band offset. Similar conclusions were found earlier by Janotti et al. [12].

II. Methodology

We have carried out ab-initio calculations within the generalised gradient approximation

of density functional theory. A full potential linearized augmented plane wave implementation in the WIEN2K code [15] was used by us in our calculations. We considered the systems GaN, GaP and GaAs and evaluated the electronic structure at the experimental lattice [16] constants of 4.52, 5.45 and 5.65 Å respectively. Electronic structure calculations were performed for different muffin tin radii and the reasons for this will be discussed in the text. Unless otherwise stated, the results disscussed will be for RMT= 2.3, 2.2 and 1.8 a.u for Ga in GaAs, GaP and GaN respectively. The radii for As, P and N were kept fixed at 2.3, 2.0 and 1.8 a.u. In the calculations $G_{MAX} = 12$ and RK= 7. The number of k-points used was 64 (4x4x4) for the self-consistency, while a gamma-centered grid of 8x8x8 was considered in the evaluation of the Density of states. The tetrahedron method of integration was used for the DOS calculation. The GGA PW91 approximation [5] to the exchange functional was used. An additional potential within the GGA+U [14] formalism was introduced on the Ga d states, and the changes in the electronic structure was calculated as a function of U. Further analysis has been carried out within a tight-binding model (discussed later) found to be adequate to give a good description of the electronic structure. This enables us to estimate bandgap shifts coming from various interactions. In addition plane wave pseudopotential calculations [17], have been carried out using PAW potentials [18]. A gamma centered grid of 8x8x8 k-points and GGA-PW91 approximation for the exchange have been used. Superlattices of the form $(GaX)_5/(Ga(U)X)_5$ were constructed to determine the valence and conduction band offsets introduced by U, measured with respect to the $U=0$ result. The electronic structure of the superlattices was carried out using a plane wave pseudopotential implementation within VASP [17]. A k-points grid of 6x6x1 was used. The positions of the atoms making up the superlattice were fully optimized.

III. Results and discussion

In Fig. 1 we have plotted the s, p, d projected density of states for $U=$ 0, 5 and 10 eV for GaAs. As expected the Ga $3d$ states are pushed deeper into the valence band as U is varied. The gross features of the valence band however remain unchanged. Apart from the bandgap underestimation in these calculations that we discussed earlier, another source of error in these calculations is the underestimation in the position of the semi core levels. This is a consequence of the overbinding of states that one finds in LDA-type calculations [10]. Experimentally [19], these levels are found at -17.0, -18.8 and -18.9 eV inside the valence band for GaN, GaP and GaAs.

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There are however some striking effects on the bandgap as U is varied. Considering the example of GaAs, one examines the variation in the bandgap as the position of the semi core states are varied (Fig. 2). The bandgap increases from 0.44 eV to 0.71 eV as U is increased from 0 to 9 eV. The first question is why does the bandgap change as the Ga $3d$ states are pushed deeper into the valence band. This is illustrated schematically in Fig. 3 for the symmetries involved at the Γ point. The energy splitting of the Ga $3d$ states in the point ion limit is shown in the left panel. One has e below t_2. The t_2 states on the As interact with the t_2 states of Ga $3d$ and hence form bonding and antibonding states. The VBM position in the absence of Ga $3d$-As p interaction would have been where the unperturbed As p derived t_2 states are. The interaction leads to a reduction in the bandgap of the semiconductor. Now as the Ga $3d$ states are pushed deeper into the valence band, one expects the VBM to stop moving at some point where the interaction strength becomes negligibly small.

In order to understand this further we have considered a minimal tight-binding model with s,p and d states in the basis for both Ga and As, P. In the case of GaN only s,p states were included on N. Nearest neighbor interactions between the anion and cation as well as next neighbor interactions between anion pairs and cation pairs have been considered. The comparisons of the band dispersions obtained for GaAs, GaP and GaN from VASP and from TB fitting for the various U values are given in Fig.4. The parameters entering the TB Hamiltonian (Table I) have been extracted by fitting the first principle results by a least square error minimization process. The parameters are similar to values present in the literature [20]. We use the values of the interactions strengths estimated between the semi-core and valence states to estimate the renormalization of the bandgap due to these interactions. This is found to be just 0.1 eV for GaAs and GaP and 0.15 eV for GaN.

Now as the Ga $3d$ states are pushed deeper into the valence band, one expects the VBM to stop moving at some point where the interaction strength becomes negligibly small. We have moved the Ga $3d$ states to absurdly deep energies using say a U of 20 eV where we expect the interaction to go to zero. The VBM however does not stop moving. A possible reason for this is the following and is shown schematically in Fig. 5. The introduced potential in the GGA+U [14] formalism is on the Ga d admixture in the ground state charge density contained within the sphere of specified mufin tin radius. This does not distinguish between Ga $3d$ and $4d$. Hence since the ground state charge density has some Ga $4d$ admixture, the Ga $4d$ states are also pulled to lower energies. These interact with the VBM derived As p

levels and hence modify the bandgap which keeps on increasing with U. This is illustrated in Fig. 6 where we show the valence and conduction band structure as U is varied. With U the changes in the valence band are small, while the changes in the conduction band are substantial. Therefore we clarify for the first time that a part of the observed increase in the bandgap with U on the semi core states is because of the interaction of the unoccupied Ga $4d$ states with the states comprising the VBM.

The question we asked next was whether we can reduce the component of the $4d$ states on which the potential is applied. This has been done by varying the muffin tin radius about the atom on which the potential is applied and the resulting density of states for GaAs are shown in Fig.7. For $U=0$ we find that the large RMT result indicates that there is substantial Ga d admixture in the valence band. However as the muffin tin radius is reduced, this contribution is substantially reduced. Hence for large U and large RMT we find the unusual result that the Ga d states contribution in the valence band increases. We would expect it to decrease by virtue of the fact that we are moving the Ga $3d$ states deeper. For small RMT however we do not find an increase in the Ga d component in the valence band. The modifications in the bandgap with RMT are given in Table II. The changes are small for small RMT, though the bandgap improvement is still larger than what is expected from the tight binding model. We examine what the modifications of the electronic structure are as a function of U with a smaller muffin tin radius of 1.5 a.u. Aligning the different U calculations with respect to the anion $1s$ for the same U, we find that the relative separtion of the anion core levels remain unchanged while those of the Ga core levels are strongly modified. This is given in Table III. From this we infer that there is no charge transfer taking place between Ga and X. However the charge on the Ga gets reorganised between the levels resulting in a change in the relative separations of the core levels. This observation is consistent with the fact that there are modifications of the charge on the Ga atoms, while that on the anions is essentially unchanged. Hence as a function of U, there are changes in the Ga-d-anion-p interactions which results in substantial modifications of the bandgap. However there is no change in the effective charge transfer between the anion and cations sites as function of U. Constructing a superlattice of the form $(GaX)_5/(Ga(U)X)_5$ we determine the valence band and conduction band offsets between the $U=0$ and finite U results. Here the value U has been chosen so that we obtain agreement in the position of the experimental Ga $3d$ positions. These are shown in Fig. 8. We find that a U on the semicore state shifts the

conduction band minimum as well as the valence band maximum to different extends. These conclusions are similar to those obtained by Janotti et al. [12].

In contrast to the LAPW method where the region over which the GGA+U correction is applied is controlled by the choice of the muffin tin radius, such a freedom does not exist in pseudopotential calculations. We have calculated the change in the bandgap for the GaN, GaP and GaAs within a pseudopotential approach (Table IV). The results are similar to our large RMT results.

In Fig. 9 we have plotted the variation of the approximate position of the Ga $3d$ states with respect to the VBM as a function of U. The behaviour is almost linear and we use this plot to determine the value of U that will bring about agreement with experiment for the Ga $3d$ states. Hence a U of approximately 11, 14 and 13 eV, with a muffin tin radius of 1.5 a.u, for GaN, GaP and GaAs respectively is found to be sufficient to bring about agreement with experiment. Similar range of U was required to get the position of the d states correct in ZnO [21]. We would however like to point out that GGA+U is basis set dependent and therefore the U value (for obtaining a certain effect) differs between different computational methods, different choice of muffin-tin radius, etc.

In Fig. 10 we have plotted the variation in the band structure of the valence band as well as the conduction band region for GaAs as a function of U for a smaller muffin tin radius of 1.5 a.u. The conduction band minimum has been defined as the zero of the energy scale. There are k dependent changes in the electronic structure that one finds. A popular method used in the correction of the band-gap of semiconductors is one in which all the states are rigidly shifted [22]. This method results in a constant shift of a band at all k points, which is indeed not the case as evident from Fig. 10. Hence a k-dependent self energy is intrinsic to the GGA+U approach which involves a self consistent solution of the Kohn-Sham Hamiltonian in the presence of the additional potential. This has been pointed out by Persson and Mirbt [23] who explain that LDA underestimates the Γ-point electron m_c and light-hole m_{lh} masses due to a too strong k-dependent bonding-antibonding interaction; the heavy-hole m_{hh} and spin-orbit split off m_{so} masses are in general less affected by this interaction. This LDA failure is very apparant for GaAs where LDA produces a very small bandgap, and the corresponding LDA average masses (see Ref. [24] for definition of the geometric average masses) are $m_c = 0.01m_0$, $m_{hh} = 0.49m_0$, $m_{lh} = 0.02m_0$, and $m_{so} = 0.07m_0$, whereas the experimental values [25] are $m_c = 0.07m_0$, $m_{hh} = 0.53\text{-}0.59m_0$, $m_{lh} =$

$0.08m_0$, and $m_{so} = 0.13m_0$. The k-dependent modifications in the GGA+U formalism result in an increase of the bandgap and also a weakening of the bonding-antibonding interaction, thereby improving the effective masses. Using the LAPW method with $U = 9$ eV we obtain $m_c = 0.04m_0$, $m_{hh} = 0.62m_0$, $m_{lh} = 0.05m_0$, and $m_{so} = 0.12m_0$ which agree much better with the measured values.

IV. Conclusion

To conclude, we have examined a popular and computationally inexpensive method of correcting for the bandgap underestimation in first-principle calculations. For small values of U one finds that the changes in the valence band are confined to the region around the Γ point. Suprisingly there are changes induced in the unoccupied states as well, as a function of U on the semi-core states. This has been pointed out as arising from the fact that the GGA+U potential is applied on the d admixture in the ground state charge density. This can be reduced by choosing a smaller muffin tin radius for the atom to which GGA+U corrections are applied. Another component to the bandgap increase is from modified screening of the valence states as the Ga d semi-core states are pushed deeper into the valence band.

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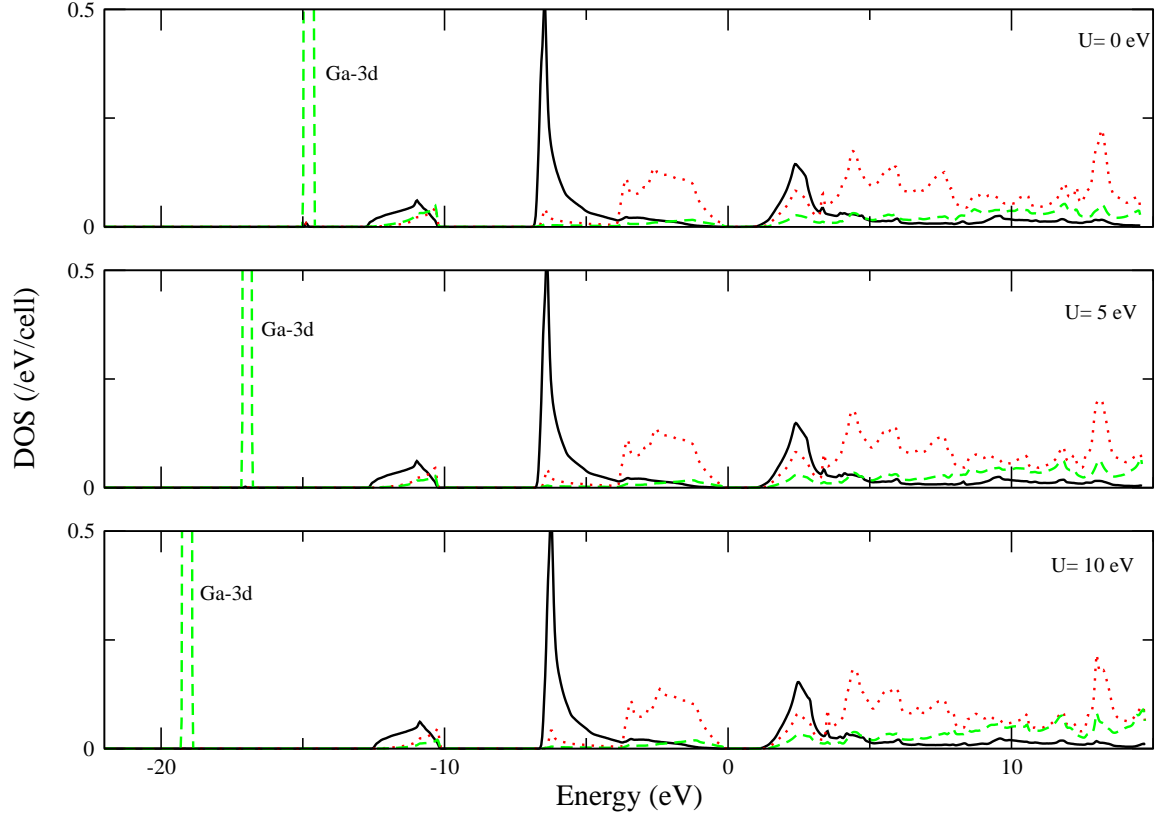[23] C. Persson and S. Mirbt, Br. J. Phys. **36**, (2006) (in press).

Fig.1. R.C,et.al

FIG. 1: The Ga - s (black solid lines), p (red dotted lines) and d (green dashed lines) projected density of states for $U=0$, 5 and 10 eV on the Ga $3d$ states for GaAs. The zero of energy corresponds to the valence band maximum.

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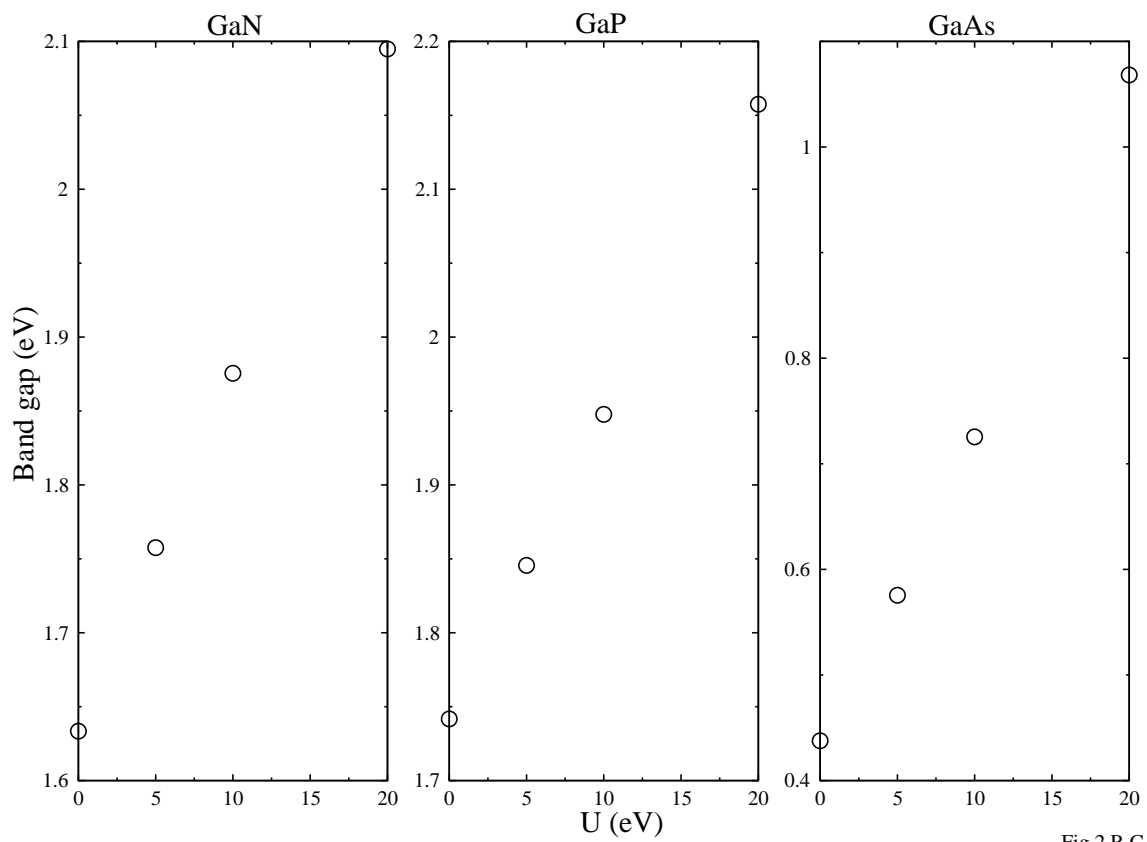
GaN   GaP   GaAs

Band gap (eV)

U (eV)

Fig.2.R.C,et al

FIG. 2: Variation of bandgap as a function of U for GaN, GaP and GaAs.

With U: reduced p-d interaction. VBM pushed to lower energies.

VBM

t_2

t_2

e

Ga 3d

As p

Fig. 3
R.C. *et al.*

FIG. 3:   Schematic energy level diagram for the interaction of the Ga 3d states with the As p states. The arrow denotes the movement of the VBM with increasing U on the semi core Ga 3d states.

GaN

GaP

Energy (eV)

GaAs

L   Γ   X   W   L   K   Γ

FIG. 4: Comparisons of the band dispersions obtained for GaN, GaP and GaAs, from ab-initio (solid lines) calculations and from TB fitting (open circles).
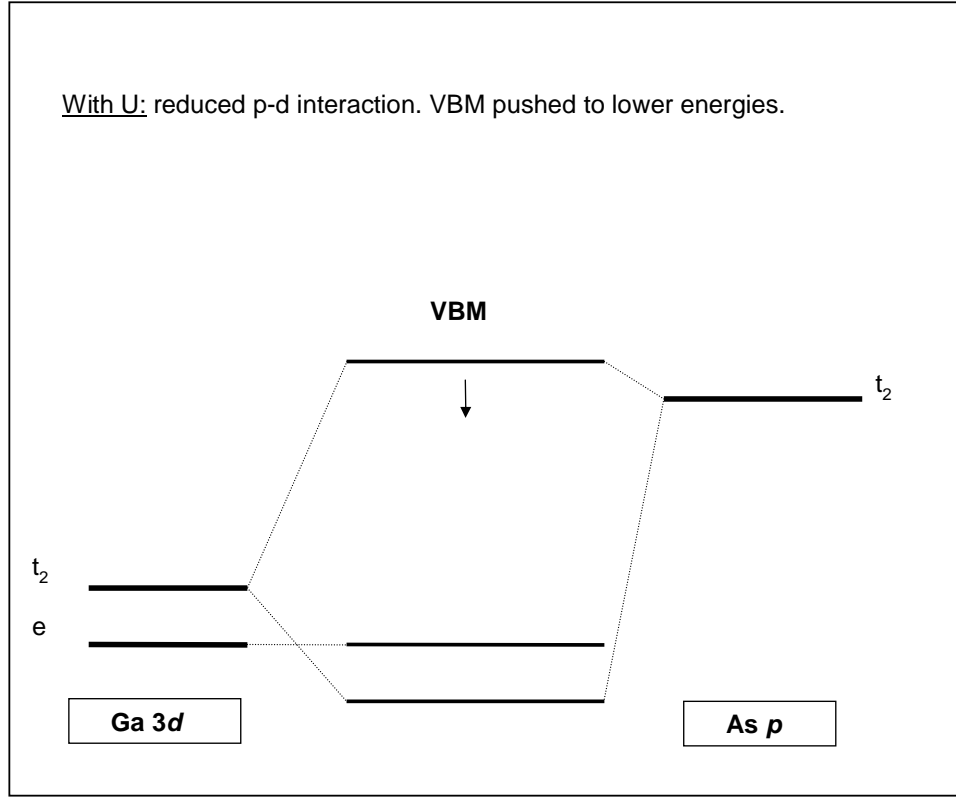
Fig. 5

R.C. *et al.*

FIG. 5: Schematic energy level diagram for the interaction of the Ga $4d$ states with the As p states. The arrow denotes the movement of the VBM with increasing U on the semi core Ga $3d$ states.
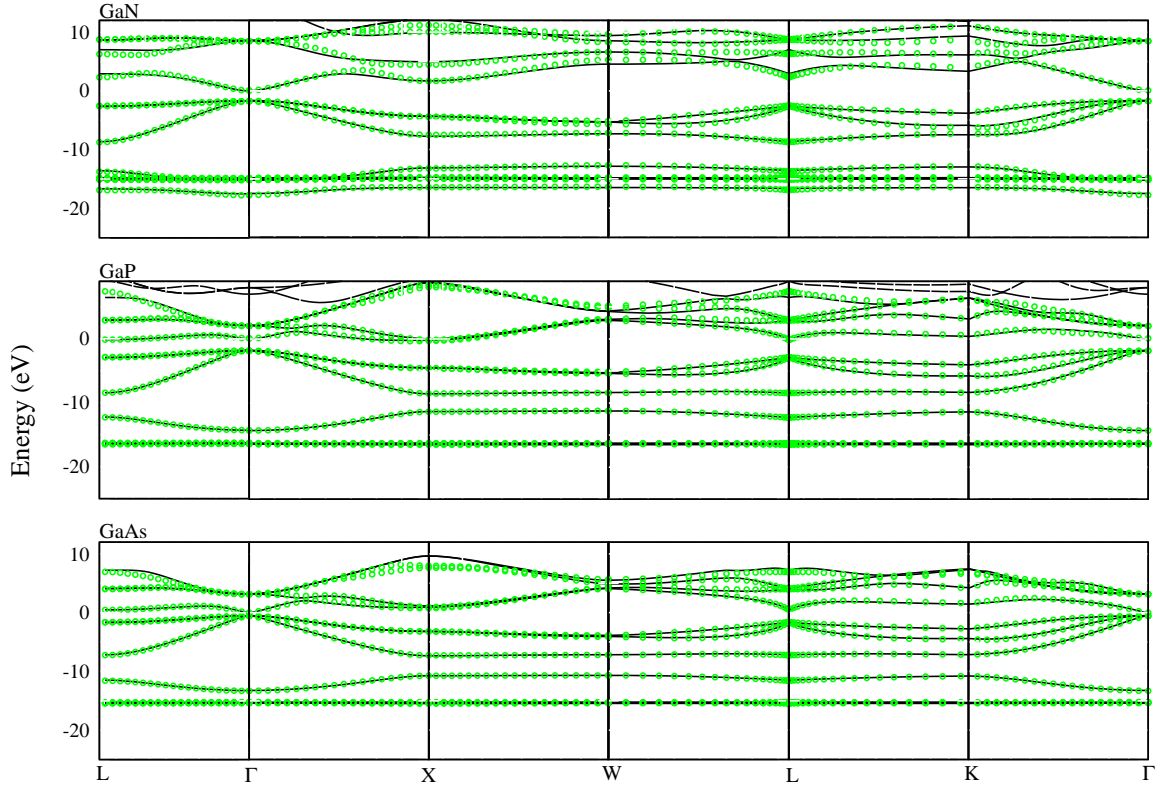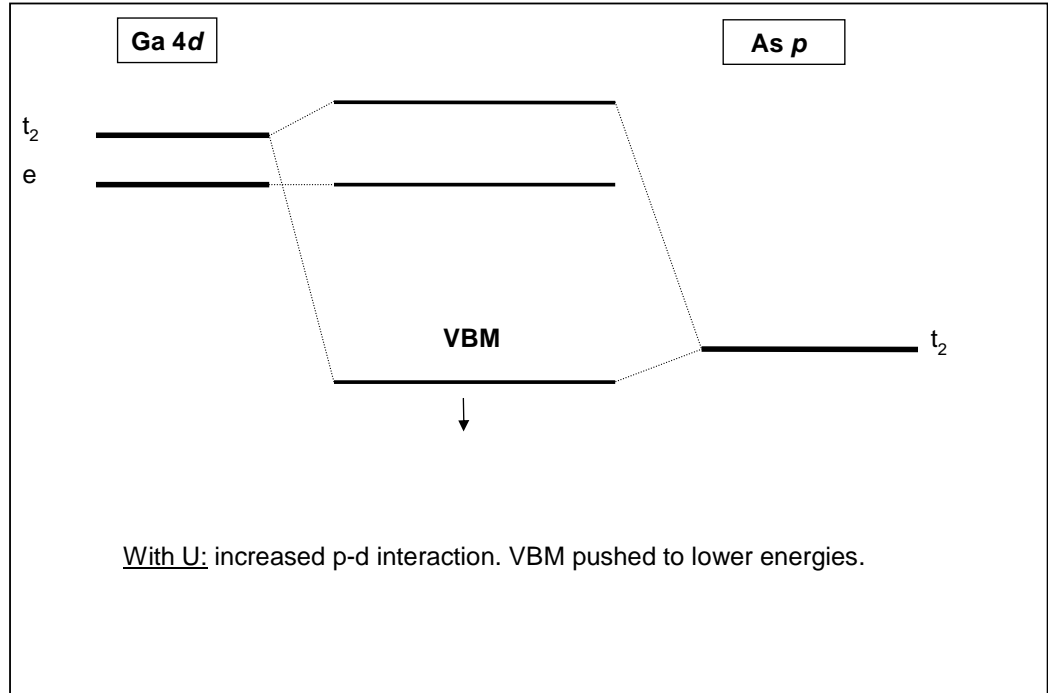
(a) Conduction band region

Energy (ev)

L Γ X

(b) Valence band region

Energy (eV)

L Γ X

Fig.5. R.C,et al.

FIG. 6: Near Γ point view of the band dispersions obtained for the GaAs for the U values 0(black solid lines), 5(red dashed lines) and 10(brown dotted lines) eV (a) in the conduction band region and (b) in the valence band region. The graphs have been aligned with respect to the As 1s level for each U value. (RMT of 2.3 a.u for Ga).

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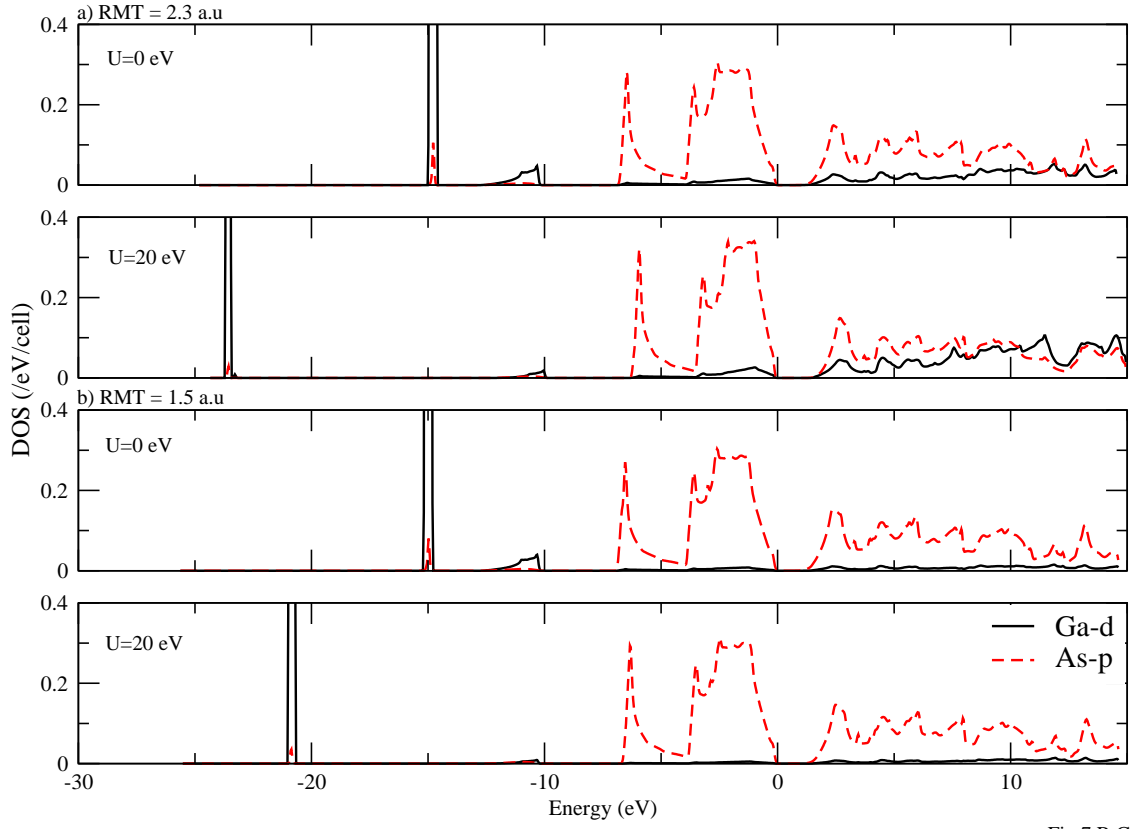
FIG. 7: The Ga d (black solid lines) and As p (red dashed lines) projected density of states for U=0 and 20 eV on the Ga 3d states for GaAs with (a) RMT= 2.3 and (b) 1.5 a.u. The zero of energy corresponds to the valence band maximum.

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(a)

GaN
U=0

Ga(U)N
U= 9 eV

E_c

0.51

1.67

E_v

0.27

2.44

13.49

17.39

Ga 3d band

4.17

(b)

GaP
U=0

Ga(U)P
U= 7 eV

E_c

0.12

1.81

E_v

0.19

2.11

14.69

17.72

Ga 3d band

3.22

(c)

GaAs
U=0

Ga(U)As
U= 10 eV

E_c

0.14

0.52

E_v

0.27

0.93

14.85

19.42

Ga 3d band

4.84
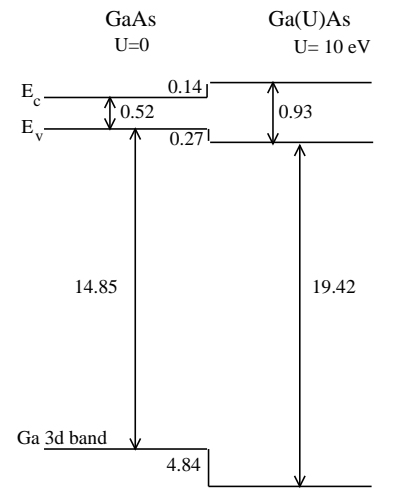
FIG. 8: Calculated band offsets at the hypothetical interfaces (a) GaN/Ga(U)N (b) GaP/Ga(U)P and (c) GaAs/Ga(U)As where a U has been introduced only on the Ga d states. PAW potentials were used for these calculations.
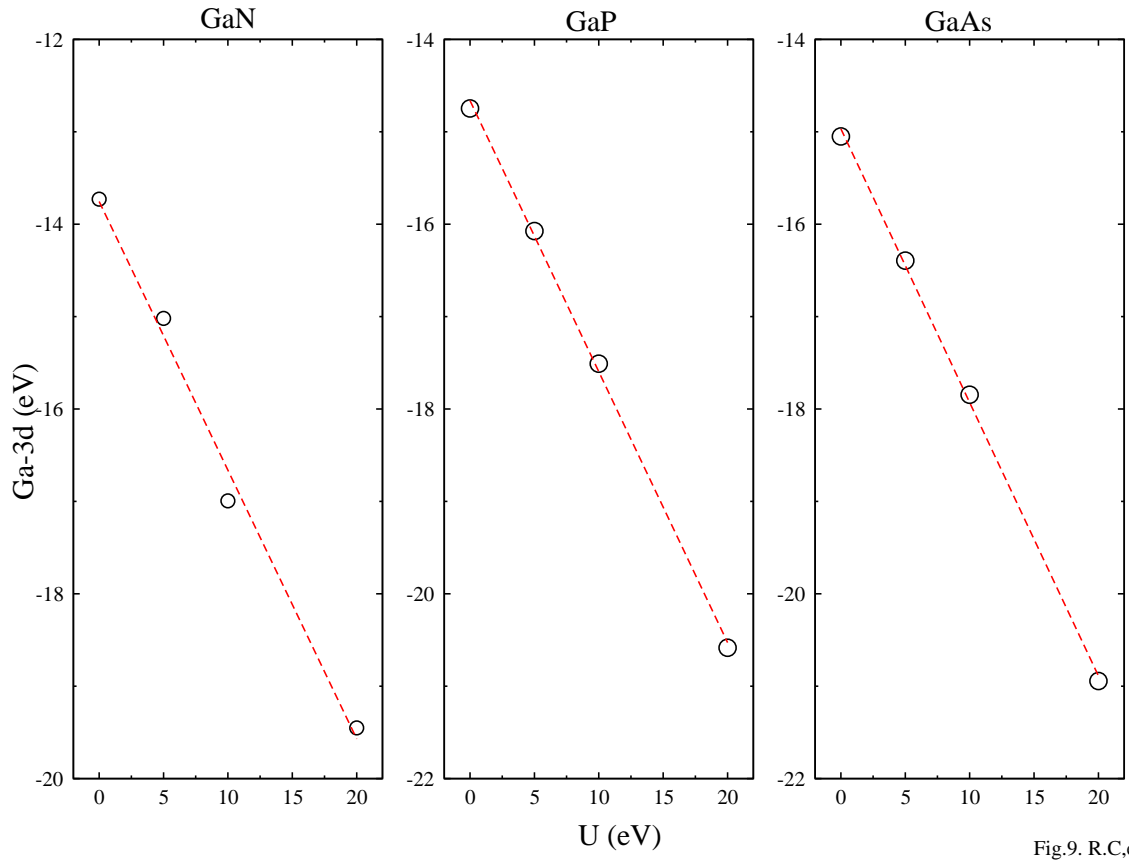
FIG. 9: Variation of Ga 3d states position with U for GaN, GaP and GaAs.

(a) Conduction band region

(b) Valence band region

Energy (eV)

Energy (eV)

U=0 eV
U=10 eV
U=20 eV

W   L   K   Γ   X
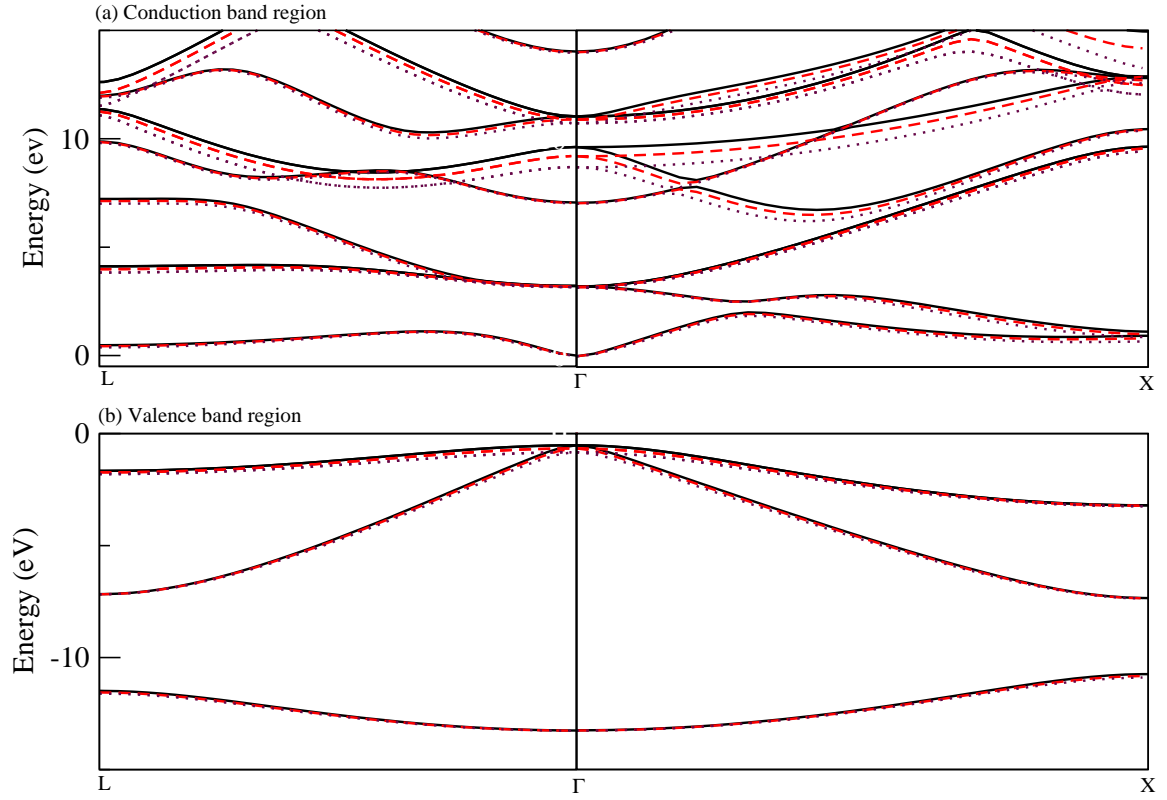
Fig.10. R.C,et al.

FIG. 10: Band dispersions obtained for the GaAs for the U values 0(black solid lines), 10(red dashed lines) and 20(brown dotted lines) eV (a) in the conduction band region and (b) in the valence band region. The graphs have been aligned with respect to the As 1s level for each U value. (RMT of 1.5 a.u for Ga).
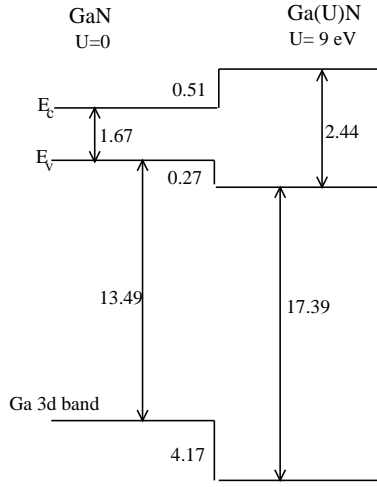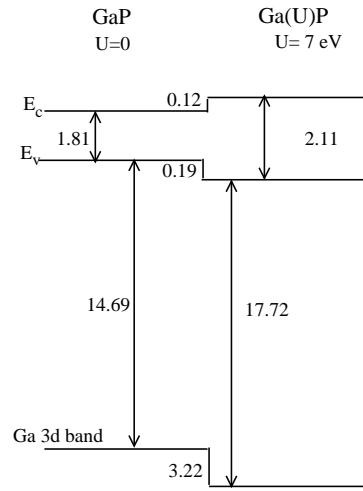
TABLE I: Tight-binding parameters (in eV) obtained from a least-squared-error fitting procedure for GaX semiconductors. The first six rows contain the orbital energies (s_c, p_c,..,d_a), where the main letter denotes orbital type (s,p,d) and the subscript denotes the cation (c) or anion (a), followed by the Slater Koster parameters. The VBM is set to the zero of the energy.

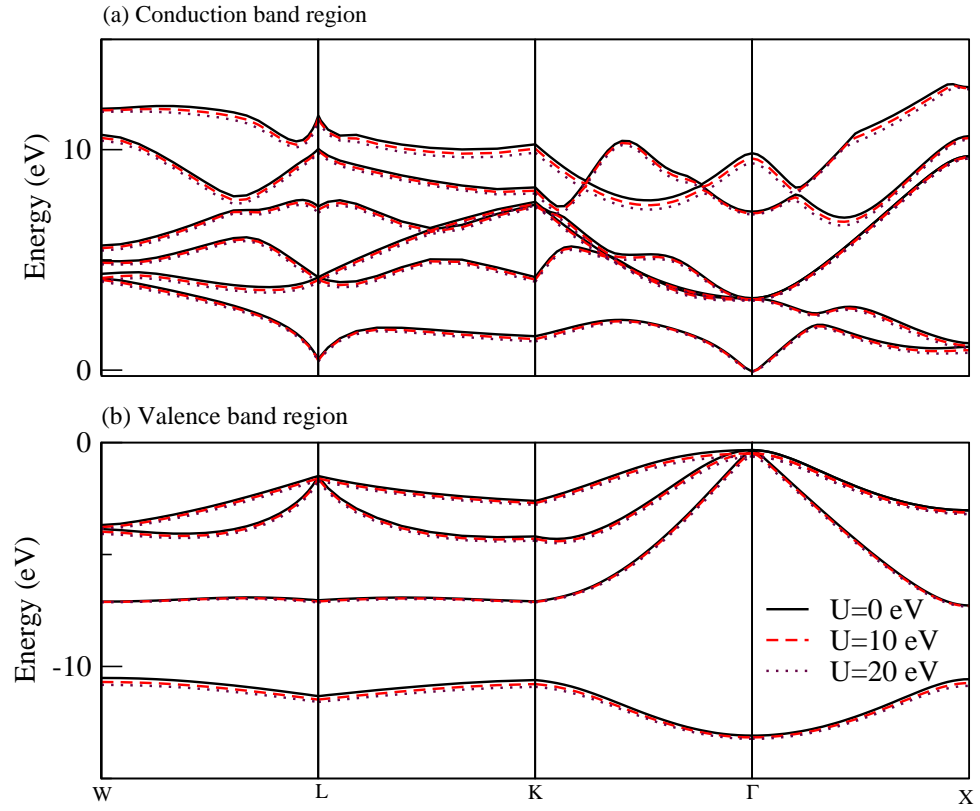|	GaN	GaP	GaAs
s_c	6.696	1.82	1.01
p_c	9.49	7.94	6.59
d_c	-13.16	-14.46	-14.74
s_a	-12.97	-8.59	-9.97
p_a	-0.92	-0.46	-0.367
d_a	-	7.71	6.88
$s_c s_a \sigma$	-1.42	-1.59	-1.33
$s_c p_a \sigma$	3.28	2.76	2.67
$s_c d_a \sigma$	-	-2.07	-1.72
$p_c p_a \sigma$	3.17	2.85	2.94
$p_c p_a \pi$	-0.92	-1.05	-0.81
$p_c d_a \sigma$	-	-0.62	-0.50
$p_c d_a \pi$	-	1.60	1.28
$d_c d_a \sigma$	-	0.0	0.0
$d_c d_a \pi$	-	0.0	0.0
$d_c d_a \delta$	-	0.0	0.0
$p_c s_a \sigma$	-0.28	-1.54	-0.75
$d_c s_a \sigma$	-0.77	0.0	0.0
$d_c p_a \sigma$	1.08	0.636	0.568
$d_c p_a \pi$	-0.01	-0.224	-0.318
$s_c s_c \sigma$	-0.59	-0.31	-0.26
$s_c p_c \sigma$	0.69	0.46	0.05
$s_c d_c \sigma$	-0.06	-0.22	-0.16
$p_c p_c \sigma$	1.49	0.11	0.28
$p_c p_c \pi$	0.0	-0.04	-0.23
$p_c d_c \sigma$	0.0	0.0	0.0
$p_c d_c \pi$	0.0	0.03	0.0
$d_c d_c \sigma$	-0.06	-0.01	0.0

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	GaN	GaP	GaAs
$d_c p_a \pi$	-0.01	-0.224	-0.318
$s_c s_c \sigma$	-0.59	-0.31	-0.26
$s_c p_c \sigma$	0.69	0.46	0.05
$s_c d_c \sigma$	-0.06	-0.22	-0.16
$p_c p_c \sigma$	1.49	0.11	0.28
$p_c p_c \pi$	0.0	-0.04	-0.23
$p_c d_c \sigma$	0.0	0.0	0.0
$p_c d_c \pi$	0.0	0.03	0.0
$d_c d_c \sigma$	-0.06	-0.01	0.0
$d_c d_c \pi$	0.02	0.01	0.01
$d_c d_c \delta$	0.0	0.0	0.0
$s_a s_a \sigma$	-0.06	0.0	-0.01
$s_a p_a \sigma$	0.2	0.0	0.07
$s_a d_a \sigma$	-	-0.15	-0.13
$p_a p_a \sigma$	0.34	0.23	0.31
$p_a p_a \pi$	-0.05	-0.05	-0.04
$p_a d_a \sigma$	-	-0.24	-0.31
$p_a d_a \pi$	-	0.15	0.13
$d_a d_a \sigma$	-	-0.98	-0.84
$d_a d_a \pi$	-	0.51	0.43
$d_a d_a \delta$	-	-0.1	-0.036

TABLE II: Bandgap change (E_g(U=20)-E_g(U=0)) as a function of muffin tin radii.

	RMT (a.u)	Bandgap change (eV)
GaN	1.8	0.46
GaN	1.5	0.34
GaP	2.0	0.42
GaP	1.5	0.29
GaAs	2.3	0.63
GaAs	1.5	0.29

TABLE III: The relative shifts on the Ga and X (anion) core levels (Ry.) with respect to the X $1s$ core level. (RMT of 1.5 a.u for Ga).

		Core level	U (eV)	
			10	20
GaN				
	Ga	$1S_{1/2}$	-723.683948	-723.581975
	Ga	$2S_{1/2}$	-64.611804	-64.501480
	Ga	$2P_{1/2}$	-53.981829	-53.871907
	Ga	$2P_{3/2}$	-51.947788	-51.837825
	Ga	$3S_{1/2}$	17.218648	17.295227
	Ga	$3P_{1/2}$	20.651111	20.725591
	Ga	$3P_{3/2}$	20.912098	20.985360
	N	$1S_{1/2}$	0.0	0.0
GaP				
	Ga	$1S_{1/2}$	-598.619678	-598.517630
	Ga	$2S_{1/2}$	60.447143	60.558034
	Ga	$2P_{1/2}$	71.077537	71.187967
	Ga	$2P_{3/2}$	73.111528	73.222006
	Ga	$3S_{1/2}$	142.286256	142.362896
	Ga	$3P_{1/2}$	145.719349	145.793838
	Ga	$3P_{3/2}$	145.980772	146.054018
	P	$1S_{1/2}$	0.0	0.0
	P	$2S_{1/2}$	140.426058	140.424829
	P	$2P_{1/2}$	144.012722	144.011600
	P	$2P_{3/2}$	144.080163	144.079036

		Core level	U (eV)	
			10	20
GaAs				
	Ga	$1S_{1/2}$	109.385718	109.544887
	Ga	$2S_{1/2}$	768.448458	768.620852
	Ga	$2P_{1/2}$	779.078965	779.250701
	Ga	$2P_{3/2}$	781.112945	781.284749
	Ga	$3S_{1/2}$	850.307135	850.427101
	Ga	$3P_{1/2}$	853.741405	853.858096
	Ga	$3P_{3/2}$	854.003530	854.118328
	As	$1S_{1/2}$	0.0	0.0
	As	$2S_{1/2}$	752.001092	752.000418
	As	$2P_{1/2}$	763.627530	763.626944
	As	$2P_{3/2}$	766.316562	766.315964
	As	$3S_{1/2}$	847.269176	847.268283
	As	$3P_{1/2}$	851.175282	851.174383
	As	$3P_{3/2}$	851.544909	851.544006

TABLE IV: Bandgap as a function of U from VASP

	U (eV)	Bandgap (eV)
GaN	0	1.633
GaN	5	1.758
GaN	10	1.875
GaN	20	2.095
GaP	0	1.742
GaP	5	1.846
GaP	10	1.948
GaP	20	2.157
GaAs	0	0.438
GaAs	5	0.576
GaAs	10	0.725
GaAs	20	1.068